

10/537,409

(FILE 'HOME' ENTERED AT 19:06:49 ON 04 MAR 2007)

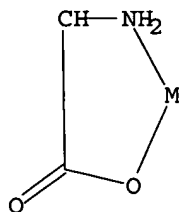
FILE 'REGISTRY' ENTERED AT 19:06:57 ON 04 MAR 2007

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1 full

FULL SEARCH INITIATED 19:07:20 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 94095 TO ITERATE

100.0% PROCESSED 94095 ITERATIONS

17762 ANSWERS

SEARCH TIME: 00.00.01

L2 17762 SEA SSS FUL L1

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

172.10

172.31

FILE 'CAPLUS' ENTERED AT 19:07:28 ON 04 MAR 2007

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FILE COVERS 1907 - 4 Mar 2007 VOL 146 ISS 11

FILE LAST UPDATED: 2 Mar 2007 (20070302/ED)

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=> s l2/prep

6919 L2

4368397 PREP/RL

L3 2510 L2/PREP  
(L2 (L) PREP/RL)

=> s l3 and py<2002  
21881904 PY<2002

L4 2113 L3 AND PY<2002

=> s l4 and amino acid chelate  
1107837 AMINO  
4322568 ACID  
45252 CHELATE  
260 AMINO ACID CHELATE  
(AMINO(W)ACID(W)CHELATE)

L5 15 L4 AND AMINO ACID CHELATE

=> d 1-15 bib abs

L5 ANSWER 1 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2002:73201 CAPLUS

DN 136:340800

TI Metal complexes of biologically important ligands, CXL. Half-sandwich complexes of ruthenium(II), rhodium(III), iridium(III) and palladium(II), platinum(II) complexes with N,O-chelates of fluorine- and thiophene-containing  $\alpha$ -amino acids

AU Koch, Daniela; Beck, Wolfgang

CS Dep. Chemie, Ludwig-Maximilians-Universitat, Munchen, D-81377, Germany

SO Zeitschrift fuer Naturforschung, B: Chemical Sciences (2001),  
56(12), 1271-1280

CODEN: ZNBSEN; ISSN: 0932-0776

PB Verlag der Zeitschrift fuer Naturforschung

DT Journal

LA German

OS CASREACT 136:340800

AB (o-Fluorophenyl)glycine and -alanine or 2-thienylglycine and -alanine react with dinuclear, chloro-bridged metal complexes to give chiral N,O-chelates (arene)M(Cl)(NH<sub>2</sub>CHRCO<sub>2</sub>) (M = Ru, Rh, Ir, arene = cymene, Cp\*) and (R3P)(Cl)M(NH<sub>2</sub>CHRCO<sub>2</sub>) (M = Pd, Pt) as mixts. of diastereoisomers or cis/trans-isomers, resp. The complexes prepared from 2-thienylglycine were diastereoselective, affording diastereoisomer or cis-trans ratios of 62:38 to 85:15.

RE.CNT 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2001:262302 CAPLUS

DN 135:76975

TI Metal complexes of biologically important ligands. Part CXXXIII.  $\alpha$ -Amino carboxylate chelates of cyclometalated rhodium complexes

AU Bohm, Andreas; Polborn, Kurt; Beck, Wolfgang

CS Department Chemie, Ludwig-Maximilians-Universitat, Munchen, D-81377, Germany

SO Zeitschrift fuer Naturforschung, B: Chemical Sciences (2001),  
56(3), 293-296

CODEN: ZNBSEN; ISSN: 0932-0776

PB Verlag der Zeitschrift fuer Naturforschung

DT Journal

LA German

OS CASREACT 135:76975

AB The Cl-bridged complexes [(2-phenylpyridine-C,N)2RhCl]2 and [(benzo[h]quinoline-C,N)2RhCl]2 react with the anions of alanine, valine, and phenylalanine to give the chiral, octahedral N,O-chelates L2Rh( $\alpha$ -amino carboxylate) as mixts. of two diastereoisomers. The complex (benzo[h]quinoline-C,N)2Rh[(S)-NH<sub>2</sub>CHMeCO<sub>2</sub>-N,O] was characterized by x-ray diffraction. Its crystals contain two diastereoisomers in the

unit cell.

RE.CNT 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 1998:318661 CAPLUS  
DN 129:75501  
TI Novel trigonal-bipyramidal copper(II) complexes containing one discrete amino acid chelate: crystal structures of [Cu(L-val)(pmdt)]ClO<sub>4</sub> and [Cu(aiba)(pmdt)]ClO<sub>4</sub>·H<sub>2</sub>O (L-val = L-valinate ion, aiba = α-aminoisobutyrate ion, and pm<sub>dt</sub> = N,N,N',N',N'-pentamethyldiethylenetriamine)  
AU Murakami, Tasuku; Kita, Shouichi  
CS Faculty of Education, Iwate University, Morioka, 020, Japan  
SO Inorganica Chimica Acta (1998), 274(2), 247-250  
CODEN: ICHAA3; ISSN: 0020-1693  
PB Elsevier Science S.A.  
DT Journal  
LA English  
AB [Cu(L-val)(pmdt)]ClO<sub>4</sub> and [Cu(aiba)(pmdt)]ClO<sub>4</sub>·H<sub>2</sub>O (L-val = L-valinate ion, aiba = α-aminoisobutyrate ion, and pm<sub>dt</sub> = N,N,N',N',N'-pentamethyldiethylenetriamine) mixed-ligand Cu(II) complexes were characterized by x-ray crystallog. These complexes take on a trans (Oamino acid, Ncentral of pm<sub>dt</sub>) form, and their CuN<sub>4</sub>O core geometries are approx. regular trigonal bipyramidal, which is novel for Cu(II) complexes containing a discrete amino acid chelate ring.

RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 1996:256860 CAPLUS  
DN 124:359191  
TI Metal amino acid chelate  
IN Hsu, Hsinhung J.  
PA J.H. Biotech, Inc., USA  
SO U.S., 8 pp.  
CODEN: USXXAM  
DT Patent  
LA English  
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5504055	A	19960402	US 1994-213263	19940315 <--
PRAI	US 1994-213263		19940315		
OS	MARPAT 124:359191				

AB A water soluble metal amino acid chelate was prepared by adding a metal salt to deaerated water, mixing the salt solution with a mixture of an amino acid and an organic acid and adjusting the pH of the resulting composition to a range of from .apprx.4.5 to .apprx.8.5 to produce a clear solution The resultant clear solution can then be applied to plants or it can be dried for storage. The water soluble metal amino acid chelate produced by the process, when applied to plants, results in increased metals assimilation and improved plant growth.

L5 ANSWER 5 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 1994:121269 CAPLUS  
DN 120:121269  
TI Organometallic ferroelectric liquid crystals. II. Syntheses, characterization and mesogenic properties of amino-acid chelated-palladated azine, azo and imine mononuclear complexes  
AU Huang, Dejian; Xiong, Nuyun; Yang, Jun; Wang, Shumei; Li, Guangnian; Zhang, Liangfu

CS Chengdu Inst. Org. Chem., Acad. Sin., Chengdu, 610015, Peop. Rep. China  
 SO Molecular Crystals and Liquid Crystals Science and Technology, Section A:  
 Molecular Crystals and Liquid Crystals (1993), 231, 191-8  
 CODEN: MCLCE9; ISSN: 1058-725X  
 DT Journal  
 LA English  
 AB Six mononuclear ortho-palladated complexes containing amino-  
 acid chelate ligands and azine or azo, imine ligands  
 were synthesized and characterized by elemental anal., IR, <sup>1</sup>H NMR and <sup>13</sup>C  
 NMR. Their thermotropic behaviors and mesogenic properties were studied.  
 The relation between mesogenic properties and mol. structures of complexes  
 were also discussed. As a result, 3 novel organometallic ferroelec. liquid  
 crystals were found.

L5 ANSWER 6 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 1989:219070 CAPLUS  
 DN 110:219070  
 TI Preparation of pharmaceutical-grade amino acid chelates free of  
 interfering anions  
 IN Ashmead, Harvey Harold  
 PA Albion International, Inc., USA  
 SO Eur. Pat. Appl., 12 pp.  
 CODEN: EPXXDW  
 DT Patent  
 LA English  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 256645	A2	19880224	EP 1987-305813	19870701 <--
	EP 256645	A3	19881109		
	EP 256645	B1	19911211		
	R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	US 4830716	A	19890516	US 1986-882150	19860703 <--
	US 4830716	B1	19991207		
	AT 70259	T	19911215	AT 1987-305813	19870701 <--
	ES 2037715	T3	19930701	ES 1987-305813	19870701 <--
	JP 63079859	A	19880409	JP 1987-165546	19870703 <--
	JP 2547026	B2	19961023		
	CA 1299812	C	19920428	CA 1987-541185	19870703 <--
PRAI	US 1986-882150	A	19860703		
	EP 1987-305813	A	19870701		

OS MARPAT 110:219070  
 AB Pharmaceutical-grade amino acid or peptide chelates, free of interfering  
 anions, are prepared by reacting an anion-free ligand (selected from  
 naturally occurring amino acids, dipeptides, tripeptides, or  
 tetrapeptides) in an aqueous reaction medium with a metal source (selected  
 from metals, metal oxides, hydroxides, and carbonates) where the metal is  
 selected from Ca, Cu, Fe, Mg, Mn, Zn, Mo, Co, Se, and V, and where the  
 metal:ligand molar ratio is  $\geq 2:1$ , and recovering the chelate. To  
 83 parts H<sub>2</sub>O was added 2 parts citric acid and 13 parts glycine, followed  
 by 2 parts Mg turnings. The mixture was set aside for 48 h, and 8 parts  
 citric acid was added. The reaction mixture was heated to 100° and  
 spray dried to produce a Mg diglycine chelate powder having Mg content  
 .apprx.10%.

L5 ANSWER 7 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 1986:637299 CAPLUS  
 DN 105:237299  
 TI Chiral metal complexes. 21. Stereochemical analysis of ternary  
 ruthenium(II) complexes of  $\alpha$ -diimines and glycine or N-substituted  
 glycines, including the crystal structure of racemic bis(2,2'-  
 bipyridine)glycinatoruthenium perchlorate dihydrate  
 AU Anderson, Malcolm A.; Richards, John P. G.; Stark, Allison G.; Stephens,  
 Frederick S.; Vagg, Robert S.; Williams, Peter A.

CS Dep. Phys., Univ. Coll., Cardiff, CF1 1XL, UK  
 SO Inorganic Chemistry (1986), 25(27), 4847-51  
 CODEN: INOCAJ; ISSN: 0020-1669  
 DT Journal  
 LA English  
 AB Photolabile rac-[RuL2(aa)]ClO4.nH2O (L = 2,2'-bipyridine (bpy) or 1,10-phenanthroline and Haa = glycine (Hgly), N-methylglycine, or N-phenylglycine) were prepared and their structures in solution analyzed by 200-MHz 1H NMR spectroscopy. The results are compared with the solid-state structure of rac-[Ru(bpy)2(gly)]ClO4.2H2O, which was determined by x-ray diffraction. This anal. is used to demonstrate the torsional effects of glycine substitution on the structure of the amino acid chelate ring, and on the nature of the diastereomeric ratios in the synthetic product mixts. Photoequilibration has allowed a quant. estimate of the discriminatory effects resulting from substitution at the N(amine) chiral centers. In the N-methylglycine chelates those diastereomers that avoid steric interaction between the CH3 group and L are selected, whereas the N-phenylglycine chelates show stereospecific coordination for the same steric reason. Both the amine and methylene protons of the coordinated amino acids exchange for deuterons at high pD. rac-[Ru(bpy)2(gly)]ClO4.2H2O, is triclinic, space group P.hivin.1, a 9.487(2), b 12.294(3), c 13.041(3) Å, α 111.36(2), β 63.15(2), γ 113.33(2), R = 0.033 and R' = 0.035 for 3752 unique reflections. The mol. structure has Ru-O = 2.105(3) and Ru-N(amine) = 2.135(4) Å with the amino acid chelate ring adopting a flattened δ conformation in the Δ enantiomer. The 4 Ru-N(bpy) bond lengths are not equivalent, the bond trans to Ru-O being significantly shorter (2.008(4) Å) than the other 3 (average Ru-N = 2.046(6) Å).

L5 ANSWER 8 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 1986:542169 CAPLUS  
 DN 105:142169  
 TI Electrochemical production of pure amino acid chelates  
 IN Ashmead, Harvey H.  
 PA Albion Laboratories, Inc., USA  
 SO U.S., 6 pp.  
 CODEN: USXXAM

DT Patent  
 LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4599152	A	19860708	US 1985-738065	19850524 <--
	EP 202936	A1	19861126	EP 1986-303886	19860522 <--
	EP 202936	B1	19930728		
	R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
	CA 1272350	A1	19900731	CA 1986-509696	19860522 <--
	AT 92038	T	19930815	AT 1986-303886	19860522 <--
	JP 62026254	A	19870204	JP 1986-117662	19860523 <--
PRAI	US 1985-738065	A	19850524		
	EP 1986-303886	A	19860522		
OS	MARPAT 105:142169				
GI					

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Amino acid chelates (I, II, III, IV, V; M = bivalent metal cation and R = radical of naturally occurring amino acid) essentially free of anion radicals other than OH and anions of weak organic acids are prepared in an electrolytic cell having anode and cathode compartments divided by a

cation permselective membrane. The amino acid chelate consists of a metal ion selected from the group consisting of Fe, Zn, Mn, Mg, Cu, Ca, and their mixts. chelated to  $\geq 1$  ligands selected from the group consisting of  $\alpha$ -amino acids, protein hydrolyzates, polypeptides, and their combinations. Pure forms of amino acid chelates are desirable for administration to biol. systems to increase the bioavailability of the metal. Thus, to the anode compartment of an electrolytic cell having a cathode and anode compartment separated by a permselective membrane (Nafion) was added an aqueous 20% glycine solution. The catholyte solution was 1% citric acid solution. 5 V d.c. at 27 A was applied across the cell for 1 h. A blue precipitate, shown to be Cu glycine chelate containing 6% Cu and a ligand to Cu ratio of 2:1, was formed. The resulting precipitate was free of any anions.

L5 ANSWER 9 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1984:603226 CAPLUS

DN 101:203226

TI Chiral metal complexes. 12. Chiroptical, proton NMR and crystallographic studies of the diastereoisomers  $\Lambda$  and  $\Delta$ -[Ru(diimine)<sub>2</sub>(S-threonine)]<sup>+</sup> and their S-allothreonine analogs

AU Goodwin, Terence J.; Williams, Peter A.; Stephens, Frederick S.; Vagg, Robert S.

CS Dep. Chem., Univ. Coll., Cardiff, CF1 1XL, UK

SO Inorganica Chimica Acta (1984), 88(2), 165-81

CODEN: ICHAA3; ISSN: 0020-1693

DT Journal

LA English

AB The 4 catatropic  $\Delta$ ,  $\Lambda$ -[RuL<sub>2</sub>(aa)]ClO<sub>4</sub>.nH<sub>2</sub>O (I) (L = 2,2'-bipyridine (bpy), 1,10-phenanthroline (phen), Haa = S-threonine, S-allothreonine) were isolated and each complex resolved into its 2 diastereoisomeric forms. Each isomer is photolabile, equilibrating to a definite  $\Lambda/\Delta$  ratio on light irradiation, with the resultant equilibrium consts. reflecting chiral discrimination energies between isomeric pairs. Equilibration of these species was followed both by CD (in H<sub>2</sub>O) and 1H NMR (in D<sub>2</sub>O) techniques. I (L = bpy, Haa = S-threonine) is monoclinic, space group P2<sub>1</sub> with a 10.165(2), b 28.220(6), c 10.896(3) Å,  $\beta$  104.80(2)°, Z = 4, R = 0.042. I (L = bpy, Haa = S-allothreonine) is monoclinic, space group P2<sub>1</sub> with a 10.226(4), b 27.979(4), c 10.875(2) Å,  $\beta$  104.99(2)°, Z = 4, R 0.037. A pseudo a-glide operation relates the 2  $\Delta$  and  $\Lambda$  forms in the asym. unit of each structure. The amino acid chelate rings in the 4 mol. structures have like conformations, suggesting only minor differences in steric factors within these cations. Evidently in the crystal structures of the S-allothreonine complexes, an internal H-bond may exist between the  $\beta$ -OH and carboxylic groups which would be unfavorable in the S-threonine complexes. This structural difference in the 2 amino acid side chains is consistent both with observed differences in the NMR spectra of the complexes, and with the different equilibration ratios obtained.

L5 ANSWER 10 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1984:482937 CAPLUS

DN 101:82937

TI Complexes with diastereoisomeric ligands. IV. The problem of stereoselectivity in amino acidatobis(chelate)cobalt(III) complexes. (Chelate = ethylenediamine, 1,10-phenanthroline, or 2,2'-bipyridyl)

AU Pasini, Alessandro

CS Dip. Chim. Inorg. Metallorg., Univ. Milano, Milan, I-20133, Italy

SO Gazzetta Chimica Italiana (1983), 113(11-12), 793-7

CODEN: GCITA9; ISSN: 0016-5603

DT Journal

LA English

AB [Co(en)<sub>2</sub>L]Cl<sub>2</sub> (HL = (S)-serine, (S)-threonine, (S)-glutamic acid, (S)-valine, [Co(bpy)<sub>2</sub>L]Cl<sub>2</sub> (bpy = 2,2'-bipyridine, HL = (S)-serine),

[Co(phen)2L]Cl2 (phen = 1,10-phenanthroline; HL = (S)-serine, (S)-valine), and  $\Lambda$ -[Co(en)2L]I2 (HL = (S)-serine) were prepared. The  $\Lambda$ : $\Delta$  ratio of these complexes was calculated from the intensity of the CD spectra. Very little or no stereoselectivity was observed. The results are discussed in terms of the amino acid chelate ring conformation.

- L5 ANSWER 11 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 1980:614627 CAPLUS  
DN 93:214627  
TI Synthesis and spectral characterization of the mixed-ligand complexes [N-(2-pyridylmethyl)-L-aspartato][amino acidato]cobalt(III), Co(PLASP)(AA)  
AU Meiske, Larry A.; Angelici, Robert J.  
CS Dep. Chem., Iowa State Univ., Ames, IA, 50011, USA  
SO Inorganic Chemistry (1980), 19(12), 3783-9  
CODEN: INOCAJ; ISSN: 0020-1669  
DT Journal  
LA English  
AB A series of mixed-ligand Co(III) complexes of the form Co(PLASP)(AA), where PLASP2- is the tetradentate ligand N-(2-pyridylmethyl)-L-aspartate and AA- is a bidentate amino acidate ligand, were prepared from Co(II) and Co(III) reactants. For the amino acidate ligands glycinate,  $\alpha$ -aminoisobutyrate, L-alaninate, L-threoninate, L-prolinate, D- and L-asparaginate, D- and L-phenylalaninate, and D-, and DL-valinate, only the facial Co(III)N3O3 isomer, in which the  $\beta$ -CO2- group of PLASP2- is coordinated trans to the pyridyl group of PLASP2-, was isolated. The bidentate amino acidate is coordinated with its amino group trans to the  $\alpha$ -CO2- of PLASP2- and its  $\alpha$ -CO2- group trans to the secondary amino N atom of PLASP2-. The CD spectra of the Co(PLASP)(AA) complexes were resolved into contributions from the optically active portion of the amino acidate chelate ring and from the rest of the mol. The latter contribution is constant for all the complexes studied. 1H NMR spectra of the complexes are also examined in terms of the conformation of the amino acidate chelate ring. In addition, visible and 13C NMR spectra of the complexes are discussed.
- L5 ANSWER 12 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 1980:614583 CAPLUS  
DN 93:214583  
TI Mixed chelate compounds of palladium(II) with  $\alpha$ -amino acids  
AU Vicol, Olga; Repede, S.; Lascar, V.  
CS Dep. Inorg. Anal. Chem., Polytech. Inst., Iasi, Rom.  
SO Buletinul Institutului Politehnic din Iasi, Sectia 2: Chimie si Inginerie Chimica (1980), 25(3-4), 17-21  
CODEN: BPICDV; ISSN: 0254-7104  
DT Journal  
LA English  
AB The complexes PdLL' and [Pd(HL)(HL')][PdCl4] (HL = alanine; HL' = glycine, valine) were prepared and characterized by chemical anal. and IR spectra.
- L5 ANSWER 13 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 1980:454833 CAPLUS  
DN 93:54833  
TI Metal complexes of amino acids. XII. The deuteration of  $\alpha$ -hydrogen atoms in cobalt(III) complexes containing  $\alpha$ -amino carboxylates  
AU Ama, Tomoharu; Kawaguchi, Hiroshi; Kanekiyo, Makoto; Yasui, Takaji  
CS Fac. Sci., Kochi Univ., Kochi, 780, Japan  
SO Bulletin of the Chemical Society of Japan (1980), 53(4), 956-60  
CODEN: BCSJAS; ISSN: 0009-2673  
DT Journal  
LA English  
AB The 2nd-order rate consts. (rate =  $k_D(\text{base})[\text{Complex}][\text{OD-}]$ ) for the D exchange of  $\alpha$ -methylene or  $\alpha$ -methine protons in the amino carboxylato complexes trans(O)-, C1-cis(O)-, and C2-cis(O)-[Co(gly)2(en)]+

and  $[\text{Co}(\text{gly})_2(\text{tn})]^+$ ,  $[\text{Co}(\text{gly})(\text{NH}_3)_4]^{2+}$ ,  $[\text{Co}(\text{gly})(\text{en})_2]^{2+}$ ,  $[\text{Co}(\text{gly})(\text{tn})_2]^{2+}$ ,  $[\text{Co}(\text{sar})(\text{en})_2]^{2+}$  and  $\Delta$ - and  $\Delta$ - $[\text{Co}(\text{L-ala})(\text{en})_2]^{2+}$  where tn is trimethylenediamine and sar is sarcosinato, were determined by the  $^1\text{H-NMR}$  measurement. The major factors determining the deuteration

rate of  $\alpha$ -H in the amino carboxylate chelate are the geometry and charge of the complex and the nature of the substituent bonded to the chelate ring to be deuterated; the minor factor is the chelate-ring size of the ligands other than amino carboxylate in a complex mol.

L5 ANSWER 14 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1978:518619 CAPLUS

DN 89:118619

TI Formation constants of mixed ligand complexes involving ligands of biological importance. pH-Metric studies of aqueous solution equilibria between nickel(II)/zinc(II)/cadmium(II), histidine, and  $\alpha$ -alanine/phenylalanine

AU Malik, G. S.; Singh, S. P.; Tandon, J. P.

CS Chem. Dep., Jat Vedic Coll., Baraut, India

SO Journal fuer Praktische Chemie (Leipzig) (1978), 320(2), 324-8

CODEN: JPCEAO; ISSN: 0021-8383

DT Journal

LA English

AB Mixed chelate stability consts. were determined by pH-metric titration at ionic strength 0.1(KNO<sub>3</sub>) and 30°. The acid dissociation constant of phenylalanine is  $\text{pK} = 9.05$ . Log  $\beta_{\text{ML}2}$  values determined are: phenylalanine = HL, Ni<sup>2+</sup> 9.64, Zn<sup>2+</sup> 8.23, Cd<sup>2+</sup> 7.00; alanine = HL, Cd<sup>2+</sup> 7.46. Log  $\beta_{\text{MAL}}$  values are: Ni<sup>2+</sup>-histidine-alanine 13.47; Ni<sup>2+</sup>-histidine-Ph 12.70; Zn<sup>2+</sup>-histidine-alanine 11.21; Zn<sup>2+</sup>-histidine-phenylalanine 10.36; Cd<sup>2+</sup>-histidine-alanine 9.32; Cd<sup>2+</sup>-histidine-phenylalanine 8.52. Stability consts. were also calculated for monohydroxy complexes MAL(OH).

L5 ANSWER 15 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1970:415201 CAPLUS

DN 73:15201

TI Cleavage of amino acid esters and peptides with hydroxo-aquo(2,2',2''-triaminotriethylamine)cobalt(III) ion

AU Kimura, Eiichi; Young, Stefan; Collman, James P.

CS Dep. of Chem., Univ. of North Carolina, Chapel Hill, NC, USA

SO Inorganic Chemistry (1970), 9(5), 1183-91

CODEN: INOCAJ; ISSN: 0020-1669

DT Journal

LA English

AB Hydroxo-aquo(2,2',2''-triaminotriethylamine)cobalt(III) ion at pH 7.5 and 60° is effective in promoting the hydrolysis of amino acid esters, dipeptides, and tripeptides. The reaction is stoichiometric and specific for N-terminal amino acids as indicated by the isolation of the triaminotriethylaminecobalt(III)-amino acid chelate formed and following the appearance of the cleavage products using thin layer chromatog.

=> s 14 and metal carbonate

1717608 METAL

297749 CARBONATE

4084 METAL CARBONATE

(METAL(W) CARBONATE)

L6 0 L4 AND METAL CARBONATE

=> s 13 and metal carbonate

1717608 METAL

297749 CARBONATE

4084 METAL CARBONATE

(METAL(W) CARBONATE)



=&gt; d 1-3 bib abs

L7 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 2007:9304 CAPLUS  
 DN 146:154712  
 TI Production of chelate complexes of amino acids and oligopeptide  
 IN Zhao, Hui; Cai, Fuliu; Li, Liren  
 PA Beijing Huamei Tianyi Science and Technology Development Co., Ltd., Peop.  
 Rep. China  
 SO Faming Zhuanli Shenqing Gongkai Shuomingshu, 22pp.  
 CODEN: CNXXEV  
 DT Patent  
 LA Chinese  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	CN 1887902	A	20070103	CN 2006-10088997	20060728
PRAI	CN 2006-10088997		20060728		

AB The title chelate complexes comprise the aspartic acid-oligopeptide chelate complex shown as  $[C_8H_8O_6N_2M \cdot xH_2O]_n$ , or the glutamic acid-oligopeptide chelate complex shown as  $[C_{10}H_{12}O_6N_2M \cdot xH_2O]_n$ , wherein M is one of Ca, Mg, Zn and other bivalent transition metal elements; n (structural unit number) = 5-7; x (water mol. number) = 0-3. The chelate complexes are produced by the steps of: (1) chelating amino acid with metal oxide, metal hydroxide or metal carbonate in aqueous solution, and (2) purifying, refining, and polycondensing at 160-260°C. The chelate complexes have the advantages of high purity, stable quality, simple process and fit cost, and are suitable for mass and industrial production. The chelate complexes can be widely used in food, drink, feed or cosmetics.

L7 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 2006:1116323 CAPLUS  
 DN 145:437637  
 TI Method for producing monosodium glutamate  
 IN Peng, Qijun  
 PA Southern Yangtze University, Peop. Rep. China  
 SO Faming Zhuanli Shenqing Gongkai Shuomingshu, 9pp.  
 CODEN: CNXXEV  
 DT Patent  
 LA Chinese  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	CN 1711910	A	20051228	CN 2005-10040864	20050701
PRAI	CN 2005-10040864		20050701		

AB The title method comprises adding carbonate and/or oxide and/or hydroxide of bivalent or trivalent metal into grain fermentation broth during the fermentation procedure to form glutamate solids, filtering to collect the glutamate solids, rinsing with water, adding  $NaCO_3$  and/or  $NaOH$  solution to allow double decomposition reaction to form metal carbonate and/or oxide and/or hydroxide sediments and monosodium glutamate solution, returning the sediments to the fermentation procedure, collecting monosodium glutamate solution, decolorizing, and crystallizing to obtain purified monosodium glutamate.

L7 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 2004:493710 CAPLUS  
 DN 141:46415  
 TI Method for preparation of amino acid chelate  
 IN Park, Myung-Gyu; Choi, Mi Hee

PA MD Bioalpha Co., Ltd., S. Korea  
 SO PCT Int. Appl., 43 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004050664	A1	20040617	WO 2003-KR2674	20031205
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
	RW:	BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
	KR 2004049294	A	20040611	KR 2003-88214	20031205
	AU 2003302660	A1	20040623	AU 2003-302660	20031205
	EP 1569943	A1	20050907	EP 2003-812388	20031205
	R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
	CN 1720249	A	20060111	CN 2003-80105098	20031205
	JP 2006509787	T	20060323	JP 2004-556973	20031205
	US 2006128799	A1	20060615	US 2005-537409	20051125
PRAI	KR 2002-76803	A	20021205		
	WO 2003-KR2674	W	20031205		

OS CASREACT 141:46415

AB The present invention provides methods for preparation of metallic amino acid chelates that are elec. neutral and free of interfering ions, by reacting a metal carbonate and an acidic amino acid in an aqueous solution, and the uses of said metallic amino acid chelates. The metallic amino acid chelates can be added to a product such as medical supplies, foods, beverages, cosmetics, feeds, etc., with maintaining the stability of the product at a variety of temperature and pH ranges and also having no effect on the properties of the product, including taste and appearance. For example, CaL2 (HL = L-glutamic acid) was prepared from seaweed Ca in H2O and L-glutamic acid (1:1-1:4 ratio) at pH 4-7 and 0-100°.

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

(FILE 'HOME' ENTERED AT 16:18:29 ON 05 MAR 2007)

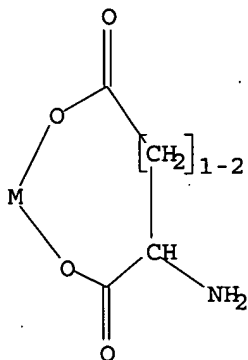
FILE 'REGISTRY' ENTERED AT 16:18:42 ON 05 MAR 2007

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 16:19:05 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 1569 TO ITERATE

100.0% PROCESSED 1569 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 29004 TO 33756

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 16:19:10 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 30486 TO ITERATE

100.0% PROCESSED 30486 ITERATIONS

45 ANSWERS

SEARCH TIME: 00.00.01

L3 45 SEA SSS FUL L1

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE ENTRY TOTAL SESSION

FULL ESTIMATED COST

172.10 172.31

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FILE LAST UPDATED: 4 Mar 2007 (20070304/ED)

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=> s 13

L4 23 L3

=> d 1-23 bib abs

L4 ANSWER 1 OF 23 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 2005:702580 CAPLUS  
DN 144:339112  
TI Determination of stability constant of glutamate zinc by indirect determination of FAAS with ZnS  
AU Liu, Wen-han; Zhang, Dan; Li, Zu-guang; Wang, Li-li  
CS College of Chemical Engineering, Zhejiang University of Technology, Hangzhou, 310014, Peop. Rep. China  
SO Guangpuxue Yu Guangpu Fenxi (2005), 25(6), 968-970  
CODEN: GYG FED; ISSN: 1000-0593  
PB Beijing Daxue Chubanshe  
DT Journal  
LA Chinese  
AB Based on indirect determination of glutamic acid by flame atomic absorption spectrometry with ZnS and the complexing action mechanism, the determination of stability constant of glutamate zinc was studied. Under the selected condition of pH 9.0, the stability constant of glutamate zinc is between  $3.3 \times 10^{20}$  and  $1.4 \times 10^{21}$ , the average value is  $\beta_W = 1.03 \times 10^{21}$ , and  $\log \beta_W = 21.013$ .

L4 ANSWER 2 OF 23 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 2003:846195 CAPLUS  
DN 140:413031  
TI pH-metric and spectrophotometric study of oxovanadium(IV) with aspartic acid, glutamic acid and imidazoles  
AU Patel, R. N.; Soni, V. K.; Sharma, S.; Shukla, K. K.; Pandeya, K. B.  
CS Department of Chemistry, A. P. S. University, Rewa, 486 003, India  
SO Oxidation Communications (2003), 26(3), 358-367  
CODEN: OXCODW; ISSN: 0209-4541  
PB SciBulCom Ltd.  
DT Journal  
LA English  
AB The equilibrium in the systems  $VO_2^{+} + A + B$  (A - aspartic or glutamic acid, B - imidazole, 2-methylimidazole and 2-ethylimidazole) have been studied at 25° C and  $\mu = 0.1$  M  $NaClO_4$  medium by a combination of pH potentiometric and spectroscopic methods (EPR and visible absorption). The results of potentiometric and spectroscopic studies are self-consistent. The stabilities of the ternary complexes follow the order: aspartic acid  $\geq$  glutamic acid with respect to amino acids and 2-methylimidazole  $\approx$  2-ethylimidazole  $>$  imidazole with respect to imidazoles. These orders have been explained in terms of electronic and mol. structures.

RE.CNT 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD

## ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 23 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 2003:413886 CAPLUS  
 DN 139:12253  
 TI Prevention or treatment of hypomagnesemia in pediatric patients and in patients with G-tubes or NG-tubes  
 IN McMains, Michael B.; Geppert, Caren D.; Siegel, Missy L.  
 PA USA  
 SO U.S. Pat. Appl. Publ., 3 pp.  
 CODEN: USXXCO  
 DT Patent  
 LA English  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2003099723	A1	20030529	US 2001-988104	20011119
	US 6579905	B2	20030617		
PRAI	US 2001-988104		20011119		

AB A method of preventing or treating hypomagnesemia in pediatric patients and patients with G-tubes or NG-tubes comprising the step of administering a pharmaceutical composition comprised of a magnesium salt, magnesium-L-aspartate hydrochloride, in a water-soluble powder concentrate  
 When dissolved in water, the pharmaceutical composition provides a method for preventing or treating hypomagnesemia in such patients without compromising the absorption or efficacy of the pharmaceutical composition

L4 ANSWER 4 OF 23 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 2002:528702 CAPLUS  
 DN 137:272347  
 TI Homo and hetero-nuclear chromium(III) complexes with natural ligands. Part 1. Spectroscopic and mass spectra studies on ternary [M-L1-L2] systems  
 AU Maciejewska, Gabriela; Cieslak-Golonka, Maria; Staszak, Zbigniew; Szelag, Adam  
 CS Institute of Inorganic Chemistry and Metallurgy of Rare Elements, University of Technology, Wroclaw, 50-370, Pol.  
 SO Transition Metal Chemistry (Dordrecht, Netherlands) (2002), 27(5), 473-480  
 CODEN: TMCHDN; ISSN: 0340-4285  
 PB Kluwer Academic Publishers  
 DT Journal  
 LA English  
 OS CASREACT 137:272347  
 AB Seven new ternary mono- and polynuclear Cr(III) complexes with natural ligands: glycine, glutaminic, nicotinic and aspartic acids, cysteine and glutathione, were isolated and physicochem. characterized. Four of them were tested and are nontoxic. The complexes were analyzed using spectroscopic (diffuse reflectance UV-visible, IR, FIR), magnetic methods, and (some) by FAB mass spectra. Spectral analyses with the digital filter and band deconvolution methods were also presented.  
 RE.CNT 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 23 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 1999:734705 CAPLUS  
 DN 132:101926  
 TI Preparation and characterization of mixed ligand complexes M(ASP)(L).H2O. M = Hg(II) and Pb(II), ASP = DL-Aspartic acid, L = 2,2'-bipyridil and 1,10-phenanthroline  
 AU Ehsan, M. Q.  
 CS Department of Chemistry, University of Dhaka, Dhaka, 1000, Bangladesh  
 SO Dhaka University Journal of Science (1999), 47(2), 263-265  
 CODEN: DJOSEM; ISSN: 1022-2502  
 PB Dhaka University Journal of Science

DT Journal  
LA English  
AB Hg and Pb complexes of DL-aspartic acid with 2,2'-bipyridine and 1,10-phenanthroline have been prepared  
RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 23 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 1999:631582 CAPLUS  
DN 132:227292  
TI Spectroscopic and thermal behavior of complex compounds useful for magnesium supplementation  
AU Wagner, Claudia C.; Ferrer, Evelina G.; Baran, Enrique J.  
CS Centro de Quimica Inorganica (CEQUINOR), Facultad de Ciencias Exactas, Universidad Nacional de La Plata, La Plata, 1900, Argent.  
SO Acta Farmaceutica Bonaerense (1999), 18(1), 5-12  
CODEN: AFBODJ; ISSN: 0326-2383  
PB Colegio de Farmaceuticos de la Provincia de Buenos Aires  
DT Journal  
LA English  
AB Synthesis of 3 Mg(II) complexes potentially useful for Mg supplementation in human and veterinary medicine is reported: Mg chloroaspartate,  $\text{Mg}(\text{C}_4\text{H}_6\text{O}_4\text{N})\text{Cl} \cdot 3\text{H}_2\text{O}$ ; Mg citrate,  $[\text{Mg}(\text{H}_2\text{O})_6][\text{MgC}_6\text{H}_5\text{O}_7(\text{H}_2\text{O})]2.5\text{H}_2\text{O}$ , and Mg orotate,  $[\text{Mg}(\text{C}_5\text{H}_3\text{O}_4\text{N}_2)_2] \cdot 8\text{H}_2\text{O}$ . These compds. were characterized by IR and Raman spectroscopy and their thermal behavior was investigated by thermogravimetric measurements and DTA, working in an O<sub>2</sub> atmospheric  
RE.CNT 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 23 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 1995:935784 CAPLUS  
DN 124:21636  
TI Effect of magnesium aspartate hydrochloride on transportation and slaughtering stress in pigs  
AU Ehrenberg, A.; Helbig, J.  
CS Research Department, Verla Pharm, Tutzing, Germany  
SO Magnesium 1993, [Symposium der Gesellschaft fuer Magnesiumforschung], 15th, Giessen, Sept. 21-23, 1992 (1993), Meeting Date 1992, 385-91.  
Editor(s): Golf, Sighart; Dralle, Dagmar; Vecchiet, Leonardo. Publisher: Libbey, London, UK.  
CODEN: 61ZMA6  
DT Conference  
LA English  
AB The authors examined whether the metabolic effects in pigs induced by transportation and slaughtering stress could be improved with different doses of magnesium aspartate hydrochloride (MAH) fed over different periods (40 mg magnesium/kg b.w. for 5 days and 5 mg magnesium/kg b.w. for 17 wk) and if the meat quality of pork could be improved. The prolonged administration of low-dose MAH (5 mg of magnesium per kg b.w. throughout the fattening period) was found to reduce the metabolic disorders that are typical features of porcine stress syndrome (PSS): significantly reduced activities (U/l) between controls and the 5 mg magnesium group were found in  $\alpha$ -HBDH (509.93-367.47), GLDH (2.29-3.69) and CK (10,869.43-4028.93); the activity of LDH (u/l) were diminished in tendency. The magnesium concentration in the blood of slaughtered pigs increased after high magnesium administration (1.10-1.14) and was significantly higher than in controls or the high magnesium group. The blood magnesium level in the 5 mg magnesium group was significantly lower than in controls and the 40 mg magnesium group. The improved meat quality was demonstrated by significantly higher pH value (5.83-5.92), tendentiously higher water-binding power (0.39-4.48) and lower conductivity (9.47-6.82). The structure of the mitochondria were better than in the controls. However, the short-term high-dose treatment with MAH had little effect on metabolic

changes induced by severe stress and on meat quality. The data indicate that long-term low-dose MAH administration can prevent stress-induced metabolism disorders and can improve the meat quality in pigs.

L4 ANSWER 8 OF 23 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 1994:644203 CAPLUS  
DN 121:244203  
TI Diaminoplatinum(II) complexes of glutamic acid: obvious chelating isomerization  
AU Lee, Young-A; Hong, Jongki; Jung, Ok-Sang; Sohn, Youn Soo  
CS Inorg. Chem. Lab., Korea Inst. Sci. Technol., Seoul, 136-791, S. Korea  
SO Bulletin of the Korean Chemical Society (1994), 15(8), 669-73  
CODEN: BKCSDE; ISSN: 0253-2964  
DT Journal  
LA English  
AB Coordination isomers of cis-(N-N)Pt(Glu) prepared by reaction of cis-(N-N)Pt(SO<sub>4</sub>) (N-N = 2NH<sub>3</sub>, ethylenediamine (en), (R,R)-1,2-diaminocyclohexane (DACH), N,N,N',N'-tetramethylethylenediamine (TMEDA)) with Ba glutamate in H<sub>2</sub>O were monitored and characterized by <sup>1</sup>H-NMR, <sup>13</sup>C-NMR, IR, and mass spectra. The reaction at room temperature affords the mixture of O,O'- and N,αO-chelated Pt(II) complexes. O,O'-chelate initially formed isomerized to N,αO-chelate on standing for a long time or at increasing temperature. The ratio of the two isomers at room temperature depends on the nature of N donor coligand (N-N).

L4 ANSWER 9 OF 23 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 1994:586971 CAPLUS  
DN 121:186971  
TI Magnesium L-aspartates and magnesium L-aspartate hydrochloride: their constitution in the crystal and in solution  
AU Schmidbaur, H.  
CS Anorganisch-Chemisches Institut, Technische Universitaet Muenchen, Garching, D-8046, Germany  
SO Health Dis. [Proc. Int. Symp. Magnesium Trace Elem.] (1993), Meeting Date 1991, 50-8. Editor(s): Nath, R.; Gill, K. D. Publisher: Ashish Publ. House, New Delhi, India.  
CODEN: 60ILAF  
DT Conference  
LA English  
AB Dissociation equilibrium of aspartic acid in aqueous solution, metal ion complexation by aspartate ligands in aqueous solution, approaches to structure elucidation of species in solution and matrixes, structure of crystalline materials, Mg di(H aspartate) hydrates, and Mg chloride L-hydrogen aspartate trihydrate are discussed.

L4 ANSWER 10 OF 23 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 1994:563837 CAPLUS  
DN 121:163837  
TI The structure of the pharmacologically active magnesium-L-hydrogenaspartate chloride trihydrate  
AU Schmidbaur, H.; Wilkinson, D. L.; Schier, A.; Helbig, J.; Manniger, G.  
CS Anorg.-Chem. Inst., Tech. Univ. Muenchen, Garching, 85747, Germany  
SO New Journal of Chemistry (1994), 18(4), 507-10  
CODEN: NJCHE5; ISSN: 1144-0546  
DT Journal  
LA English  
AB Single crystals of the therapeutically most efficient magnesium drug with the composition Mg(L-AspH) Cl + 3H<sub>2</sub>O have been obtained upon slow evaporation of the solvent from concentrated aqueous solns. of the amorphous spray-dried material. Through determination of the structure of this compound it has been estimated that Mg(L-AspH) Cl + 3H<sub>2</sub>O is a discrete, individual phase with two

crystallog. very similar complex units. The structure features poly-cationic layers of the composition  $[Mg(L-AspH)(H_2O)_2]_n$  and intercalated  $H_2O$  mols. and  $Cl^-$  ions. In the complex units the magnesium atoms are in an octahedral environment, with bidentate anions  $L-AspH^-$  (attached through their  $\alpha$ - and  $\beta$ -carboxylate groups), two trans-hydrate water mols., and two carbonyl oxygen atoms from neighboring complex units occupying the vertices. The (protonated) amino function has no metal contact but is part of the hydrogen bonding network of the crystal.

L4 ANSWER 11 OF 23 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1992:462281 CAPLUS

DN 117:62281

TI The effect of some new platinum (II) and palladium (II) coordination complexes on rat hepatic nuclear transcription in vitro

AU Mital, R.; Shah, G. M.; Srivastava, T. S.; Bhattacharya, R. K.

CS Dep. Chem., Indian Inst. Technol., Bombay, 400 076, India

SO Life Sciences (1992), 50(11), 781-90

CODEN: LIFSAK; ISSN: 0024-3205

DT Journal

LA English

AB Several new L-amino acid derivs. of 2,2'-bipyridine and 1,10-phenanthroline complexes of platinum (Pt) and palladium (Pd) and a few binuclear 2,2'-bipyridine complexes of these metals were tested for their potential to inhibit rat hepatic nuclear transcription in vitro. Pd complexes were generally more effective inhibitors of transcription than the corresponding Pt complexes. Among Pd-diimine chlorides, the 2,2'-bipyridine complex was nearly 10 times more active than the corresponding 1,10-phenanthroline complex. Both Pt-diimine chlorides, however, showed same level of inhibitory activity. Amino acid derivs. were less inhibitory with respect to the parent metal diimine chlorides except for 1,10-phenanthroline complexes of Pd. For binuclear 2,2'-bipyridine complexes of Pt, the increase in length of linking hydrocarbon chain increased the inhibitory potential of the complex. The mechanism of inhibition of transcription by these metal complexes examined by using actinomycin-D and poly[d(I-C)] to differentiate effect on the two major components of transcription machinery viz. the template and the enzyme. These studies along with studies on the reconstituted system of transcription using either pretreated template or enzyme indicate that these metal complexes displayed dual effects on transcription by inhibiting both the template and the enzymes.

L4 ANSWER 12 OF 23 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1991:464745 CAPLUS

DN 115:64745

TI Preparation of organoplatinum antileukemia drugs

IN Talebian, Abdolhossen; Green, Dianna C.; Schein, Philip S.

PA Georgetown University, USA

SO PCT Int. Appl., 52 pp.

CODEN: PIXXD2

DT Patent

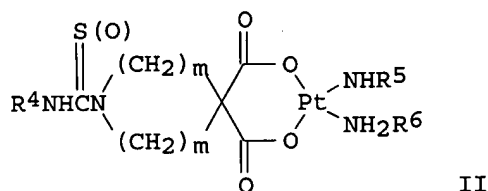
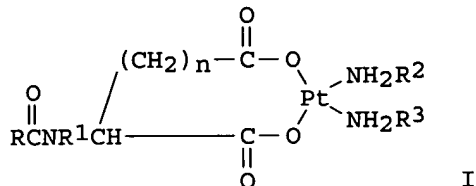
LA English

FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9008157	A1	19900726	WO 1990-US171	19900117
	W: AU, CA, HU, JP, NO, SU				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, IT, LU, NL, SE				
	US 4946954	A	19900807	US 1989-301773	19890126
	AU 9050394	A	19900813	AU 1990-50394	19900117
	ZA 9000336	A	19901031	ZA 1990-336	19900117
	EP 462980	A1	19920102	EP 1990-902930	19900117
	R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, LU, NL, SE				
	JP 04502767	T	19920521	JP 1990-503681	19900117
	JP 2771326	B2	19980702		



RU 2074861	C1	19970310	RU 1990-5001256	19900117
NO 9102732	A	19910711	NO 1991-2732	19910711
NO 180588	B	19970203		
NO 180588	C	19970514		
PRAI US 1989-297368	A	19890117		
US 1989-301773	A	19890126		
US 1987-74825	B2	19870717		
US 1988-143761	A2	19880114		
WO 1990-US171	A	19900117		
OS MARPAT 115:64745				
GI				



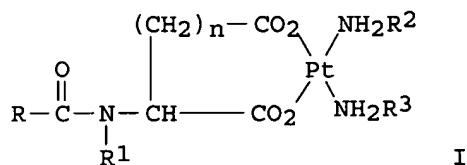
AB Due to the dicarboxylate-imparted mol. structure the chelated platinum (II) complex amine salts I and II are more water-soluble, and less damaging to kidney and bone marrow. I and II ( $n = 0$  or  $1$ ; when  $n = 1$ ,  $R_1 = H$  or  $C1-4$  alkyl,  $R = \text{alkyl}$ , mono- or disaccharide; when  $n = 0$ ,  $R_1 = H$ ,  $C1-4$  alkyl,  $R = H$ , halo, alkyl, etc.;  $R_2, R_3 = H$ ,  $C1-4$  alkyl;  $R_2R_3 = \text{fused or bicyclic}$ , or alkylene in 4-8 member ring when  $R \neq R_1 = H$  and  $n = 0$ ;  $m = 1, 2$ ;  $R_4 = \text{mono- or disaccharide}$ ;  $R_5, R_6 = H$ ,  $C1-4$  alkyl;  $CR_5R_6 = 5\text{- or }6\text{-member ring}$ ) are prepared as antileukemia drugs. Pentaacetylgluconyl chloride was reacted with iminomalononic acid in  $N,N$ -diisopropylethylamine/ $CH_3CN$  to give the iminomalononic acid intermediate, which was treated with  $Ba(OH) \cdot 2.8H_2O$  and then added to  $cis\text{-(}R,R\text{)-sulfato(cyclohexane-1,2-diamine-}N,N'\text{)platinum(II)}$  in an aqueous solution to give

the iminomalononic acid-chelated Pt-complex cyclohexanediamine salt. A dosage form suitable for i.v. administration was 130 mg active ingredient/ $m^2$  body surface of patient in an isotonic solution and in vivo tests on mice-carried P388 leukemia cells were conducted.

L4 ANSWER 13 OF 23 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 1991:440792 CAPLUS  
 DN 115:40792  
 TI Platinum pharmaceutical agents  
 IN Talebian, Abdolhossen; Green, Dianna C.; Schein, Philip S.  
 PA Georgetown University, USA  
 SO U.S., 16 pp. Cont.-in-part of U.S. Ser. No. 297,368.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4946954	A	19900807	US 1989-301773	19890126
	US 4895936	A	19900123	US 1988-143761	19880114

CA 2045120	A1	19900718	CA 1990-2045120	19900117
WO 9008157	A1	19900726	WO 1990-US171	19900117
W: AU, CA, HU, JP, NO, SU				
RW: AT, BE, CH, DE, DK, ES, FR, GB, IT, LU, NL, SE				
AU 9050394	A	19900813	AU 1990-50394	19900117
ZA 9000336	A	19901031	ZA 1990-336	19900117
EP 462980	A1	19920102	EP 1990-902930	19900117
R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, LU, NL, SE				
JP 04502767	T	19920521	JP 1990-503681	19900117
JP 2771326	B2	19980702		
HU 59690	A2	19920629	HU 1990-1456	19900117
IL 93090	A	19951031	IL 1990-93090	19900117
NO 9102732	A	19910711	NO 1991-2732	19910711
NO 180588	B	19970203		
NO 180588	C	19970514		
AU 9454792	A	19940331	AU 1994-54792	19940131
AU 674185	B2	19961212		
PRAI US 1987-74825	B2	19870717		
US 1988-143761	A2	19880114		
US 1989-297368	A2	19890117		
US 1989-301773	A	19890126		
WO 1990-US171	A	19900117		
OS MARPAT 115:40792				
GI				

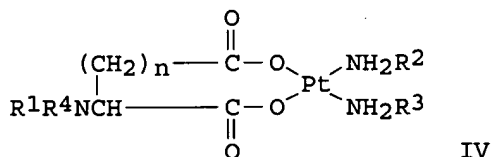
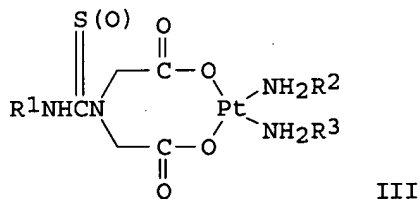
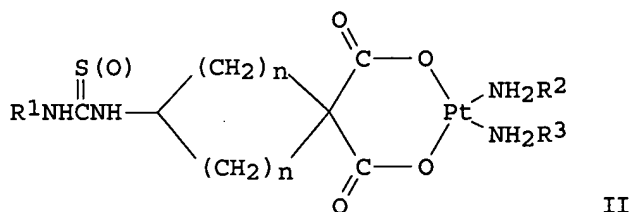
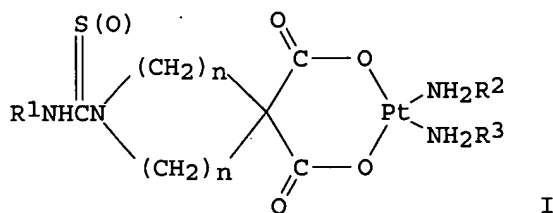


AB Pt compds. useful in the treatment of cancer are disclosed. Compns. containing these compds. and methods of using the same are also discussed, with antitumor testing data. Compds. having the formula I, where n is 0 or 1 and when n is 1, R<sup>1</sup> is H or C1-4 alkyl, R is nonsubstituted higher alkyl or mono or disaccharide or a derivative of a mono or disaccharide, when n is 0, R<sup>1</sup> is H or C1-alkyl, R is H, halogen, nonsubstituted C1-20 alkyl, aryl, aralkyloxy, mono or disaccharide, or a derivative of a mono or disaccharide, and R<sup>2</sup> and R<sup>3</sup> are selected from H, C1-4 alkyl or R<sup>2</sup> and R<sup>3</sup> or R<sup>2</sup> and R<sup>3</sup> together are linked to adjacent C atoms on a 4-, 5-, or 6-membered ring structure, or R<sup>2</sup> and R<sup>3</sup> together form a fused or bicyclic ring with adjacent C atoms, or R<sup>2</sup> and R<sup>3</sup> together are a substituted or unsubstituted C1-5 alkylene group; with the proviso that R and R<sup>1</sup> cannot both be H when n = 0, or a pharmaceutically acceptable salt thereof, are particularly useful.

L4 ANSWER 14 OF 23 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 1990:90426 CAPLUS  
 DN 112:90426  
 TI Preparation of platinum compounds for the treatment of cancer  
 IN Talebian, Abdolhossen; Green, Diana C.; Hammer, Charles F.; Schein, Philip S.  
 PA Georgetown University, USA  
 SO PCT Int. Appl., 48 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 FAN.CNT 3

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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PI	WO 8900574	A1	19890126	WO 1988-US2353	19880718
	W: AU, JP				
	RW: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
	US 4895936	A	19900123	US 1988-143761	19880114
	US 4895935	A	19900123	US 1988-143762	19880114
	AU 8821230	A	19890213	AU 1988-21230	19880718
	AU 615937	B2	19911017		
	EP 376959	A1	19900711	EP 1988-906550	19880718
	EP 376959	B1	19930324		
	R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
	JP 03500532	T	19910207	JP 1988-506291	19880718
	JP 2749092	B2	19980513		
	AT 87314	T	19930415	AT 1988-906550	19880718
	CA 1330793	C	19940719	CA 1988-572280	19880718
PRAI	US 1987-74825	A	19870717		
	US 1988-143761	A	19880114		
	US 1988-143762	A	19880114		
	EP 1988-906550	A	19880718		
	WO 1988-US2353	A	19880718		
OS	MARPAT 112:90426				
GI					



AB Pt compds. (I-III;  $n = 1, 2$ ;  $R_1$  = mono- or disaccharide or derivative thereof;  $R_2, R_3$  = C1-4 alkyl or  $R_2$  and  $R_3$  together being linked to adjacent C's on a 5- or 6-membered ring) and (IV;  $n = 0, 1$ ;  $R_1$  = H, mono- or disaccharide or derivative thereof linked to the N by NHCO, NHCS, CO;  $R_2, R_3$  = H, C1-4 alkyl; or  $R_2$  and  $R_3$  together being linked to adjacent C's on a 4-, 5- or 6-membered ring or  $R_2R_3$  forming a fused or bicyclic ring with adjacent C's;  $R_4$  = H, C1-4 alkyl; provided that  $R_1$  and  $R_4$  cannot both be H when  $n = 0$ ) useful as anticancer agents, are prepared Reaction of 3,4,6-tri-O-acetyl-2-acetamido-2-deoxyglucopyranosyl isothiocyanate with aspartic acid in aqueous MeCN containing (iso-Pr)<sub>2</sub>NEt gave 2-[[[(3,4,6-tri-O-acetyl)-2-acetamido-2-deoxy- $\alpha$ -D-glucopyranosyl)amino]thiocarbonyl]am

ino]butanedioic acid. An aqueous solution of Ba salt of the latter and cis-sulfato-1,2-cyclohexanediamine-Pt(II) (preparation given) was agitated 2 h in N in the dark to give (S)-IV [R1 = [(3,4,6-tri-O-acetyl-2-acetamido-2-deoxy- $\alpha$ -D-glucopyranosyl)amino]thiocarbonyl, R2R3 = 1,2-cyclohexylidene, R4 = H] (V). V at 400 mg/kg showed 76% increased life span (ILS) of mice implanted i.p. with 1 + 106 P388 leukemia cells vs. 96% ILS for cisplatin at 10 mg/kg.

L4 ANSWER 15 OF 23 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1989:490377 CAPLUS

DN 111:90377

TI Effects of pH and anion substitution on magnesium accumulation in rabbit aortic smooth muscle

AU Shetty, Suraj S.; Weiss, George B.

CS Res. Dep., Ciba-Geigy Corp., Summit, NJ, USA

SO Blood Vessels (1989), 26(2), 65-76

CODEN: BLVSAB; ISSN: 0303-6847

DT Journal

LA English

AB The effects of anion substitution, pH, and extracellular Mg<sup>2+</sup> concentration on 28Mg accumulation were examined in rabbit aortic smooth muscle. Accumulation of 28Mg (expressed as a 28Mg/Mg<sup>2+</sup> ratio) was not changed when the concentration of added, nonradioactive MgCl<sub>2</sub> was increased from 1.5 to 15.0 mM. The 28Mg efflux rate was increased by added MgCl<sub>2</sub> (0.15, 0.5, or 1.5 mM) in a concentration-related manner after a similar delay of 5-10 min.

Addition

of 1.5 mM MgCl<sub>2</sub>, MgSO<sub>4</sub>, or Mg aspartate HCl enhanced 28Mg efflux and inhibited accumulation of 28Mg to the same extent. An increase or decrease in extracellular pH correspondingly increased or decreased 28Mg accumulation. However, the 28Mg efflux rate was not altered when extracellular pH was decreased. Efflux of 28Mg was increased by added 1.5 mM MgCl<sub>2</sub> at pH 7.4 but not at pH 5.8. Thus, the net uptake of Mg<sup>2+</sup> appears to be proportional to the concentration of extracellular Mg<sup>2+</sup> in rabbit aorta. Low external pH decreases 28Mg retention in rabbit aorta by inhibiting the uptake of 28Mg rather than by increasing 28Mg efflux. Effects of added Mg<sup>2+</sup> on transmembrane movements of 28Mg are not altered by changes in the associated anion. Extracellular Mg<sup>2+</sup> appears to enter the cell and exchange with an intracellularly located pool of 28Mg in the same manner, regardless of whether the accompanying anion is SO<sub>4</sub><sup>2-</sup>, Cl<sup>-</sup>, or monoaspartate-HCl.

L4 ANSWER 16 OF 23 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1988:300 CAPLUS

DN 108:300

TI Synthesis, spectroscopic, mutagenic, and cytotoxicity studies of some mixed-ligand platinum(II) complexes of 2,2'-bipyridine and amino acids

AU Jain, Nidhi; Mital, Renu; Ray, K. Sen; Srivastava, T. S.; Bhattacharya, R. K.

CS Dep. Chem., IIT, Bombay, 400 076, India

SO Journal of Inorganic Biochemistry (1987), 31(1), 57-64

CODEN: JIBIDJ; ISSN: 0162-0134

DT Journal

LA English

AB Seven platinum(II) complexes of the type [Pt(bipyridine)(AA)]<sup>n+</sup> (where n = 1 or 0 and AA is the anion of L-valine, L-isoleucine, L-aspartic acid (dianion), L-glutamic acid (dianion), L-glutamine, L-proline, or S-methyl-L-cysteine) were prepared and characterized. The modes of binding of amino acids in these complexes were ascertained by IR and <sup>1</sup>H-NMR spectral studies. The L-glutamine complex inhibited in vitro P-388 leukemia cell growth by 50% at a concentration (IC<sub>50</sub>) of >20-100  $\mu$ g/mL. The IC<sub>50</sub> values for the other amino acid complexes were >100  $\mu$ g complex/mL. The above complexes were inferior at inhibiting growth of P-388 cells to platinum(II) complexes of 2,2'-bipyridine with L-alanine, L-leucine, L-methionine, and L-asparagine, as reported earlier. The platinum(II)

complexes of 2,2'-bipyridine with glycine, L-alanine, L-leucine, L-valine, L-methionine, L-phenylalanine, L-serine, L-tyrosine, and L-tryptophan were nonmutagenic on TA 100 and TA 98 bacterial strains. This is in contrast to cisplatin, which causes base pair substitution mutagenesis.

- L4 ANSWER 17 OF 23 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 1986:637349 CAPLUS  
DN 105:237349  
TI Structure elucidation of the pharmacologically active magnesium L-aspartate complexes  
AU Schmidbaur, Hubert; Mueller, Gerhard; Riede, Juergen; Manninger, Gebhard; Helbig, Joachim  
CS Anorg.-Chem. Inst., Tech. Univ. Muenchen, Garching, D-8046, Fed. Rep. Ger.  
SO Angewandte Chemie (1986), 98(11), 1014-16  
CODEN: ANCEAD; ISSN: 0044-8249  
DT Journal  
LA German  
AB Aqueous Mg(HL)2.4H2O (I; H2L = L-aspartic acid) was treated with OH- to give MgL(H2O)3 (II) which on neutralization by HCl gave Mg(HL)Cl(H2O)3 (III). II was also obtained from I and aqueous MgCl2. II is orthorhombic, space group P212121, with a 6.140(1), b 9.430(1), c 15.015(1) Å, d.(calculated) = 1.560 g cm-3, Z = 4, Rw = 0.041, R = 0.027 for 1849 reflections with I ≥ 2.0σ(I). II is octahedral with tridentate L2-. III is also octahedral but with HL- being bidentate, coordinating through the carboxylate O atoms.
- L4 ANSWER 18 OF 23 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 1986:583241 CAPLUS  
DN 105:183241  
TI Magnesium aspartate hydrochloride  
AU Weiss, George B.; Traina, Vincent M.; Douglas, Frank L.  
CS Pharm. Div., Ciba-Geigy Corp., Summit, NJ, 07901, USA  
SO New Cardiovascular Drugs (1986) 243-57  
CODEN: NCDREP; ISSN: 0891-3692  
DT Journal; General Review  
LA English  
AB A review with 55 refs. on the cardiovascular pharmacol. of Mg2+ and the pharmacol., pharmacokinetics and therapeutic activity of Mg aspartate-HCl (MAH) [91198-22-0]. The therapeutic applications of an orally effective Mg2+ salt such as MAH include frank hypomagnesemic states and as an orally effective Ca2+-like membrane stabilizer and a physiol. cellular Ca2+ antagonist.
- L4 ANSWER 19 OF 23 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 1984:416836 CAPLUS  
DN 101:16836  
TI Studies on magnesium. 1. Its pharmacological effects  
AU Kaemmerer, K.; Kietzmann, M.  
CS Inst. Pharmakol., Hannover, D-3000/71, Fed. Rep. Ger.  
SO Zentralblatt fuer Veterinaermedizin, Reihe A (1984), 31(4), 251-68  
CODEN: ZVRAAX; ISSN: 0300-8711  
DT Journal  
LA German  
AB The pharmacol. activity of Mg2+ either as Mg aspartate, MgCl2, or MgS2O3 administered orally or i.p. was compared in various expts. MgCl2 and Mg aspartate administered i.p. decreased the motility in mice, the effect was more pronounced with the latter. I.p. administered Mg preps. increased Nembutal narcosis in mice, whereas orally administered Mg preps. had no such effect. I.p. administered MgCl2 or Mg aspartate lowered normal body temperature and decreased fever induced by i.p. injected bacterial lipopolysaccharide. MgCl2 (i.p.) administered simultaneously with Neguvon (i.p.) decreased the lethal effects of Neguvon, however this was not observed with Mg aspartate. The activities of disaccharidases and leucinarylamidase in rat intestine homogenate were altered as a result of

Mg feedings when compared to controls. Protein synthesis in liver was increased in rats fed Mg aspartate, but not in rats fed MgCl<sub>2</sub> or MgSO<sub>4</sub>.

L4 ANSWER 20 OF 23 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1980:484046 CAPLUS

DN 93:84046

TI Circularly polarized luminescence studies of the ternary complexes formed between terbium(III), pyridine-2,6-dicarboxylic acid, and amino acids

AU Brittain, Harry G.

CS Dep. Chem., Seton Hall Univ., South Orange, NJ, 07079, USA

SO Journal of the American Chemical Society (1980), 102(11), 3693-8

CODEN: JACSAT; ISSN: 0002-7863

DT Journal

LA English

AB Ternary complexes formed between pyridine-2,6-dicarboxylic acid (DPA), Tb(III), and various amino acids (AA) were prepared and studied by circularly polarized luminescence (CPL) spectroscopy. The CPL spectra are reliable reporters of the bonding changes undergone by the complexes as both complex structure and solution pH were varied. Weak unipos. CPL was observed in the Tb(DPA)<sub>2</sub>(AA) system when the amino acid coordinated in a unidentate manner, while doublet-signed CPL of comparable magnitude was observed if the amino acid was able to coordinate in a bidentate manner. If the pH was raised to 8-10, a precipitate of Tb(DPA) formed and left

Tb(DPA)<sub>3</sub>(AA)

in solution. For most amino acids, double-signed CPL was observed in this pH region, the sign pattern being opposite to that seen at low pH for the bidentate amino acid chelation. This new optical activity is due to closure of a -NH<sub>2</sub>CHCOO- chelate ring after deprotonation of the amino acid ammonium group.

L4 ANSWER 21 OF 23 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1972:104685 CAPLUS

DN 76:104685

TI Thermodynamics of complex formation of indium metal ion with mercapto, hydroxy, and amino-substituted succinic acid

AU Sarin, R.; Munshi, K. N.

CS Chem. Lab., Univ. Nagpur, Nagpur, India

SO Journal of Inorganic and Nuclear Chemistry (1972), 34(2), 581-90

CODEN: JINCAO; ISSN: 0022-1902

DT Journal

LA English

AB Potentiometric studies on the free ligands and the metal complexes of In(III) with thiomalic, malic, and aspartic acid gave stepwise protonation consts. of the ligands and the formation consts. of the complexes. Thermodynamic formation consts. were obtained by extrapolation of the values at various ionic concns. The values of overall changes in  $\Delta G^\circ$ ,  $\Delta H^\circ$ , and  $\Delta S^\circ$  accompanying the reactions were determined at 35°. The trend in the stability constant values of In(III) complexes is thiomalic > malic > aspartic.

L4 ANSWER 22 OF 23 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1971:470860 CAPLUS

DN 75:70860

TI Optically active coordination compounds. XXII. Stereoselectivity in isomers of the (L-glutamate)bisethylenediaminecobalt(III) ion

AU Gillard, R. D.; Maskill, R.; Pasini, A.

CS Chem. Lab., Univ. Kent, Canterbury, UK

SO Journal of the Chemical Society [Section] A: Inorganic, Physical, Theoretical (1971), (13), 2268-70

CODEN: JCSIAP; ISSN: 0022-4944

DT Journal

LA English

AB The formation and properties of the D- and L-diastereoisomer of formula [Co(en)<sub>2</sub>(L-glut)]<sup>+</sup> (L-glutH<sub>2</sub> is L-glutamic acid), where L-glut is chelated

to Co as an  $\alpha$ -amino-acidate, have been studied. Of the many possible diastereoisomers only 4 are formed, and the stereoselectivity is kinetic in origin.

L4 ANSWER 23 OF 23 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 1971:411103 CAPLUS  
DN 75:11103  
TI Thermodynamics and stability constants of uranium-aspartic acid complex  
AU Trivedi, C. P.; Mathur, P. N.; Sunar, O. P.  
CS Dep. Chem., Univ. Jodhpur, Jodhpur, India  
SO Journal of the Indian Chemical Society (1971), 48(3), 270-2  
CODEN: JICSAH; ISSN: 0019-4522  
DT Journal  
LA English  
AB U(VI) complexes of aspartic acid as a ligand have been studied potentiometrically in aqueous media. Presence of one complex has been established. The stability constant of the complex formed was computed at 3 different temps. Log K<sub>1</sub> values were 8.34, 8.93, and 10.40 at 30, 40, and 50°, resp. The values of  $\Delta G$ ,  $\Delta H$ , and  $\Delta S$  calculated at 30° are -11.53 kcal/mole, -25.966 kcal/mole, and -47.67 cal/degree mole, resp.